

**BEST AVAILABLE COPY**

10/736,739 YONG CHU 4-21-2006

\$%^STN;HighlightOn=;HighlightOff=;

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: ssptaylc1626

**PASSWORD :**

TERMINAL (ENTER 1, 2, 3, OR ?):2

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 08:47:02 ON 21 APR 2006

FILE 'REGISTRY' ENTERED AT 08:47:14 ON 21 APR 2006  
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STRUCTURE FILE UPDATES: 19 APR 2006 HIGHEST RN 881169-11-5  
DICTIONARY FILE UPDATES: 19 APR 2006 HIGHEST RN 881169-11-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

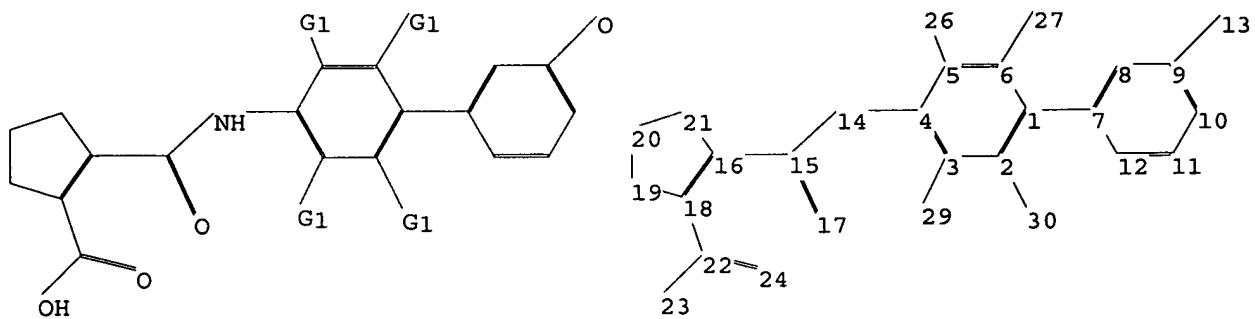
```
*****
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*****
```

Structure search iteration limits have been increased. See **HELP SLIMITS** for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

```
=> Uploading C:\Program Files\Stnexp\Queries\10736739\10736739.str
```



chain nodes :

13 14 15 17 22 23 24 26 27 29 30

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 16 18 19 20 21

chain bonds :

1-7 2-30 3-29 4-14 5-26 6-27 9-13 14-15 15-16 15-17 18-22 22-23 22-24

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 16-18 16-21

18-19 19-20 20-21

exact/norm bonds :

2-30 3-29 4-14 5-26 6-27 9-13 14-15 15-17 16-18 16-21 18-19 19-20 20-21

exact bonds :

1-7 15-16 18-22

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 22-23 22-24

G1:H,X

Match level :

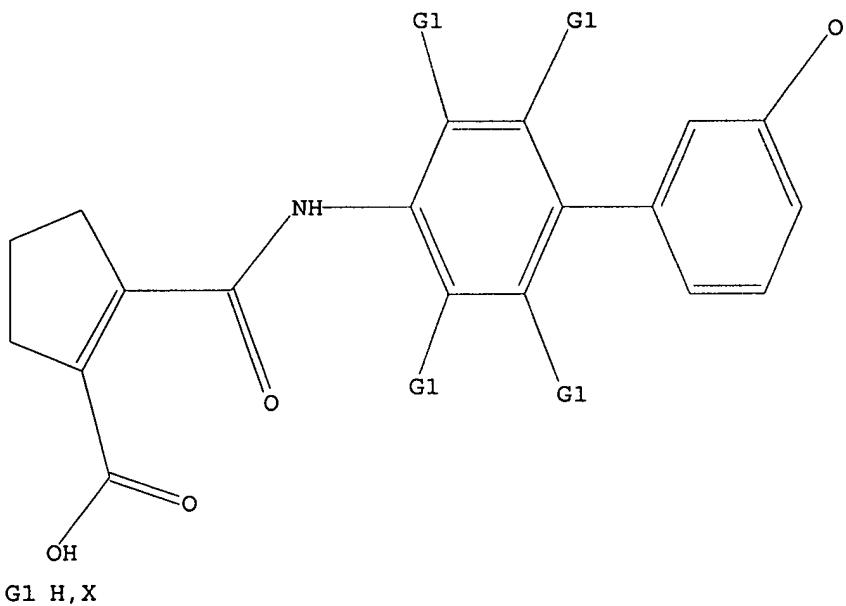
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
 11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:Atom 17:CLASS 18:Atom 19:Atom  
 20:Atom 21:Atom 22:CLASS 23:CLASS 24:CLASS 26:CLASS 27:CLASS 29:CLASS  
 30:CLASS

L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

```
=> s 11
SAMPLE SEARCH INITIATED 08:47:40 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 2 TO 124
```

L2 2 SEA SSS SAM L1

```
=> s 11 full
FULL SEARCH INITIATED 08:47:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 278 TO ITERATE
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100.0% PROCESSED 278 ITERATIONS 27 ANSWERS
SEARCH TIME: 00.00.01
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L3 27 SEA SSS FUL L1

```
=> file reg
COST IN U.S. DOLLARS SINCE FILE TOTAL
                           ENTRY SESSION
FULL ESTIMATED COST           166.94 167.15
```

```
FILE 'REGISTRY' ENTERED AT 08:47:53 ON 21 APR 2006
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```

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 19 APR 2006 HIGHEST RN 881169-11-5

DICTIONARY FILE UPDATES: 19 APR 2006 HIGHEST RN 881169-11-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
*****  
*  
* The CA roles and document type information have been removed from *  
* the IDE default display format and the ED field has been added, *  
* effective March 20, 2005. A new display format, IDERL, is now *  
* available and contains the CA role and document type information. *  
*  
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

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=> s 13
SAMPLE SEARCH INITIATED 08:48:04 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 12 TO ITERATE

100.0% PROCESSED 12 ITERATIONS 2 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                      BATCH **COMPLETE**
PROJECTED ITERATIONS: 33 TO 447
PROJECTED ANSWERS: 2 TO 124

L4 2 SEA SSS SAM L1

=> d ibib abs hitstr tot
'IBIB' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'ABS' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
'HITSTR' IS NOT A VALID FORMAT FOR FILE 'REGISTRY'
```

The following are valid formats:

Substance information can be displayed by requesting individual fields or predefined formats. The predefined substance formats are: (RN = CAS Registry Number)

REG	- RN
SAM	- Index Name, MF, and structure - no RN
FIDE	- All substance data, except sequence data
IDE	- FIDE, but only 50 names
SQIDE	- IDE, plus sequence data
SQIDE3	- Same as SQIDE, but 3-letter amino acid codes are used
SQD	- Protein sequence data, includes RN
SQD3	- Same as SQD, but 3-letter amino acid codes are used
SQN	- Protein sequence name information, includes RN
CALC	- Table of calculated properties
EPROP	- Table of experimental properties

PROP - EPROP and CALC

Any CA File format may be combined with any substance format to obtain CA references citing the substance. The substance formats must be cited first. The CA File predefined formats are:

ABS -- Abstract  
APPS -- Application and Priority Information  
BIB -- CA Accession Number, plus Bibliographic Data  
CAN -- CA Accession Number  
CBIB -- CA Accession Number, plus Bibliographic Data (compressed)  
IND -- Index Data  
IPC -- International Patent Classification  
PATS -- PI, SO  
STD -- BIB, IPC, and NCL

IABS -- ABS, indented, with text labels  
IBIB -- BIB, indented, with text labels  
ISTD -- STD format, indented

OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels

SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations

The ALL format gives FIDE BIB ABS IND RE, plus sequence data when it is available.

The MAX format is the same as ALL.

The IALL format is the same as ALL with BIB ABS and IND indented, with text labels.

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.  
HELP FORMATS -- To see detailed descriptions of the predefined formats.  
ENTER DISPLAY FORMAT (IDE):end

	SINCE FILE	TOTAL
	ENTRY	SESSION
=> file caplus		
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	1.32	168.47

FILE 'CAPLUS' ENTERED AT 08:49:29 ON 21 APR 2006  
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FILE COVERS 1907 - 21 Apr 2006 VOL 144 ISS 18  
FILE LAST UPDATED: 20 Apr 2006 (20060420/ED)

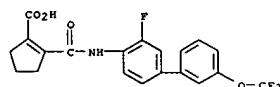
Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13  
L5 6 L3

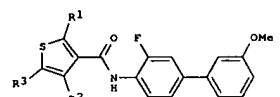
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L5 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2006:87597 CAPLUS  
 DOCUMENT NUMBER: 144:304503  
 TITLE: Dual Binding Mode of a Novel Series of DHODH Inhibitors  
 AUTHOR(S): Baumgartner, Roland; Walloschek, Markus; Kralik, Martin; Gotschlich, Astrid; Tasler, Stefan; Mies, Jan;  
 CORPORATE SOURCE: Lebán, Johann  
 SOURCE: 4SC AG, Martinsried, 82152, Germany  
 Journal of Medicinal Chemistry (2006), 49(4), 1239-1247  
 CODEN: JMCMAR; ISSN: 0022-2623  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Human dihydroorotate dehydrogenase (DHODH) represents an important target for the treatment of hyperproliferative and inflammatory diseases. In the cell DHODH catalyzes the rate-limiting step of the de novo pyrimidine biosynthesis. DHODH inhibition results in beneficial immunosuppressant and antiproliferative effects in diseases such as rheumatoid arthritis. Here, we present high-resolution X-ray structures of human DHODH in complex with a novel class of low mol. weight compds. that inhibit the enzyme in the nanomolar range. Some compds. showed an interesting dual binding mode within the same cocrystal strongly depending on the nature of chemical substitution. Measured in vitro activity data correlated with the prevailing mode of binding and explained the observed structure-activity relationship. Addnl., the X-ray data confirmed the competitive nature of the inhibitors toward the putative ubiquinone binding site and will guide structure-based design and synthesis of mols. with higher activity.  
 IT 669063-49-4 669063-57-4 669063-59-6  
 RL: PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses); (dual binding mode of novel series of DHODH inhibitors)  
 RN 669063-49-4 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-{[(3-fluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)amino]carbonyl}- (9CI) (CA INDEX NAME)

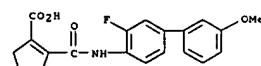


RN 669063-57-4 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-{[(3,5-difluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)amino]carbonyl}- (9CI) (CA INDEX NAME)

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1251595 CAPLUS  
 DOCUMENT NUMBER: 144:150196  
 TITLE: Biphenyl-4-ylcarbamoyl thiophene carboxylic acids as potent DHODH inhibitors  
 AUTHOR(S): Lebán, Johann; Kralik, Martin; Mies, Jan; Baumgartner, Roland; Gassen, Michael; Tasler, Stefan  
 CORPORATE SOURCE: 4SC AG, Martinsried, 82152, Germany  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(2), 267-270  
 CODEN: BMCLB8; ISSN: 0960-894X  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 144:150196  
 GI

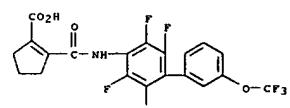


AB A previously discovered dihydroorotate dehydrogenase (DHODH) inhibitor series was further improved by replacing the cyclopentene ring by aromatic heterocycles. Different isomers of these compds., e.g. I (R1 = R2 = H; R3 = H; R1 = R3 = HO2C, R2 = H; R1 = H, R2 = R3 = HO2C), were prepared by the directed ortho-metalation procedure. The compds. are more active than the corresponding cyclopentene analogs and show potent effects on peripheral blood mononuclear cell (PBMC) proliferation.  
 IT 717824-30-1  
 RL: PAC (Pharmacological activity); BIOL (Biological study); (preparation and biol. evaluation of biphenylcarbamoyl thiophene- and furan carboxylic acids as dihydroorotate dehydrogenase inhibitors and peripheral blood mononuclear cell antiproliferative agents)  
 RN 717824-30-1 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-{[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl}- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

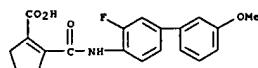
L5 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 RN 669063-59-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-{[(2,3,5,6-tetrafluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)amino]carbonyl}- (9CI) (CA INDEX NAME)



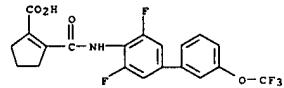
REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)

L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2005:1024942 CAPLUS  
 DOCUMENT NUMBER: 141:398883  
 TITLE: SAR, species specificity, and cellular activity of cyclopentene dicarboxylic acid amides as DHODH inhibitors  
 AUTHOR(S): Lebau, Johann; Kralik, Martin; Mies, Jan; Gassen, Michael; Tentschert, Karin; Baumgartner, Roland  
 CORPORATE SOURCE: 4SC AG, Martinistraße, 82152, Germany  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(21), 4854-4857  
 CODEN: BMCLB8; ISSN: 0960-894X  
 PUBLISHER: Elsevier B.V.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Novel DHODH inhibitors were developed based on a previously described series by introduction of heteroatoms into the cyclopentene ring and hydroxyl groups attached to it. Also, the hydrophobic biphenyl side chain was replaced with benzyloxy Ph groups. Activities on human, rat, and mouse enzymes indicate a species specificity of these inhibitors.  
 IT 717824-30-19  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses); (cyclopentene dicarboxylic acid amides as DHODH inhibitors)  
 RN 717824-30-1 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl- (9CI) (CA INDEX NAME)



IT 669063-57-4P 669063-59-6P 717824-35-6P  
 717824-36-7P 867287-88-5P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses); (cyclopentene dicarboxylic acid amides as DHODH inhibitors)  
 RN 669063-57-4 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3,5-difluoro-3'-trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl- (9CI) (CA INDEX NAME)



RN 669063-59-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(2,3,5,6-tetrafluoro-3'-

L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:550931 CAPLUS  
 DOCUMENT NUMBER: 141:99739  
 TITLE: Dihydroorotate dehydrogenase (DHODH) inhibitors and method for their identification  
 INVENTOR(S): Lebau, Johann; Kramer, Bernd; Baumgartner, Roland; Aullinger-Fuchs, Katharina; Tessler, Stefan  
 PATENT ASSIGNEE(S): 4SC A.G., Germany  
 SOURCE: PCT Int. Appl., 357 pp.  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

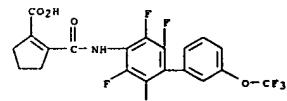
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056147	AI	20040708	WO 2003-EPI4435	20031217
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RW: BG, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG				

EP 1541198	AI	20050615	EP 2003-28137	20031205
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US 2004176458	AI	20040909	US 2003-736711	20031217
US 2004192758	AI	20040930	US 2003-736742	20031217
EP 1581478	AI	20051005	EP 2003-913575	20031217
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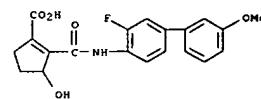
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		EP 2003-28137	A 20031205	
		US 2002-435258P	P 20021223	
		WO 2003-EPI4435	W 20031217	

OTHER SOURCE(S): MARPAT 141:99739  
 AB The present invention relates to compds. containing non-aromatic ring systems or heteroarom. ring systems, which are capable of binding to the ubiquinone binding site of DHODH. Methods for identification of such compds. are also disclosed.  
 IT 669063-49-4D, complexes with dihydroorotate dehydrogenase  
 669063-57-4D, complexes with dihydroorotate dehydrogenase  
 669063-59-6D, complexes with dihydroorotate dehydrogenase  
 717824-30-1D, complexes with dihydroorotate dehydrogenase  
 717824-35-6D, complexes with dihydroorotate dehydrogenase  
 717824-36-7D, complexes with dihydroorotate dehydrogenase  
 717824-53-8 717824-54-9 717824-57-2

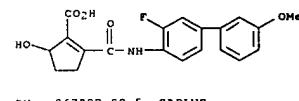
L5 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 (trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl- (9CI) (CA INDEX NAME)



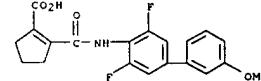
RN 717824-35-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl-3-hydroxy- (9CI) (CA INDEX NAME)



RN 717824-36-7 CAPLUS  
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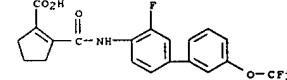
RN 867287-88-5 CAPLUS  
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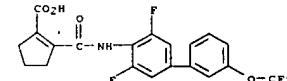
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

L5 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)  
 717824-60-7 717824-64-1 717824-86-7  
 717825-01-9 717825-16-6 717825-40-6  
 717825-46-2  
 RL: PRP (Properties)  
 (dihydroorotate dehydrogenase inhibitors and inhibitor identification method)

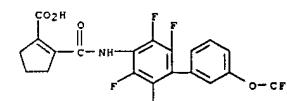
RN 669063-49-4 CAPLUS  
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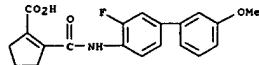
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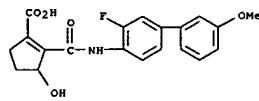
RN 669063-59-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(2,3,5,6-tetrafluoro-3'-trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl- (9CI) (CA INDEX NAME)



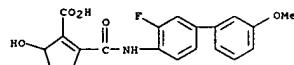
RN 717824-30-1 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl- (9CI) (CA INDEX NAME)



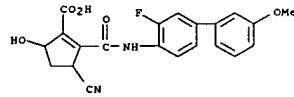
RN 717824-35-6 CAPLUS  
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 4-yl)amino]carbonyl]-3-hydroxy- (9CI) (CA INDEX NAME)



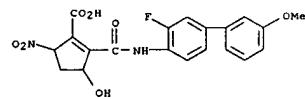
RN 717824-36-7 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid,  
 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-  
 4-yl)amino]carbonyl]-5-hydroxy- (9CI) (CA INDEX NAME)



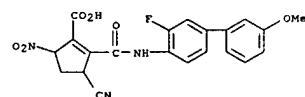
RN 717824-53-8 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 3-cyano-2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-5-hydroxy- (9CI) (CA INDEX NAME)



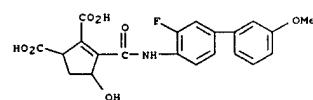
RN 717824-54-9 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid,  
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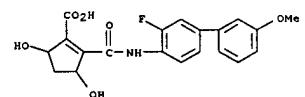
RN 717825-01-9 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 3-cyano-2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-5-nitro- (9CI) (CA INDEX NAME)



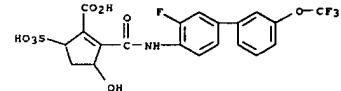
RN 717825-16-6 CAPLUS  
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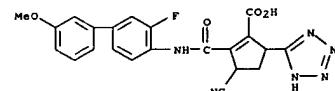
RN 717825-40-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid,  
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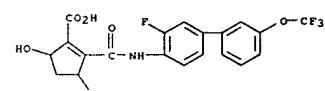
RN 717825-46-2 CAPLUS  
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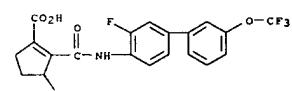
RN 717824-57-2 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 3-cyano-2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-5-(1H-tetrazol-5-yl)- (9CI) (CA INDEX NAME)



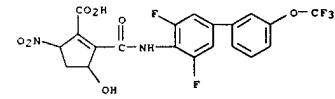
RN 717824-60-7 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid,  
 2-[(3-fluoro-3'-trifluoromethoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-3,5-dihydroxy- (9CI) (CA INDEX NAME)



RN 717824-64-1 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 3-cyano-2-[(3-fluoro-3'-trifluoromethoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 717824-86-7 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid,  
 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-3-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



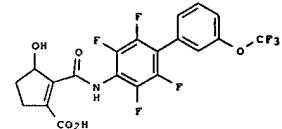
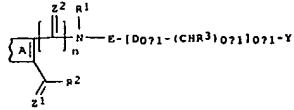
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

LS ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 2004:550930 CAPLUS  
 DOCUMENT NUMBER: 141:106198  
 TITLE: A preparation of cycloalkenedicarboxylic acid derivatives, useful as dihydroorotate dehydrogenase (DHODH) inhibitors  
 INVENTOR(S): Lebenn, Johann; Kralik, Martin  
 PATENT ASSIGNEE(S): 4SC A.-G., Germany  
 SOURCE: PCT Int. Appl., 56 pp.  
 CODEN: PIKKD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 3  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
WO 2004056746	A1	20040708	WO 2003-EPI4434	20031217	
W: AZ, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, RU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MM, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, 2M, 2W					
RW: BW, GH, GM, KE, LS, MM, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BE, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD					
TG	CA 2509138	AA	20040708	CA 2003-2509138	20031217
AU 2003299316	A1	20040714	AU 2003-299316	20031217	
US 2004176458	A1	20040909	US 2003-736711	20031217	
US 2004192758	A1	20040930	US 2003-736742	20031217	
EP 1581477	A1	20051005	EP 2003-799487	20031217	
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003017731	A	20051122	BR 2003-17731	20031217	
JP 2006511564	T2	20060406	JP 2004-561332	20031217	
PRIORITY APPLN. INFO.:			DE 2002-10260800	A 20021223	
			US 2002-435256P	P 20021223	
			WO 2003-EPI4434	W 20031217	

OTHER SOURCE(S): MARPAT 141:106198  
 GI

LS ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



AB The invention relates to a preparation of cycloalkenedicarboxylic acid derivs. of formula I [wherein: A is a non-aromatic ring containing 4 to 8 carbon atoms, wherein the ring system comprises at least one double bond and wherein one or more of the carbon atoms in the ring can be replaced by S, O, N, or S(O), etc.; D is O, S, SO<sub>2</sub>, or CH<sub>2</sub>, etc.; Z1 and Z2 are independently selected from O, S, or NH, etc.; R1 is H or alkyl; R2 is H, OH, O-(cyclo)alkyl, or NH<sub>2</sub>, etc.; R3 is H, (cyclo)alkyl, aryl, alkoxy, halogen, or O-aryl, etc.; E is an alkyl or cycloalkyl group or a (mono/poly)cyclic (un)substituted ring system; Y is H, halogen, haloalkyl, haloalkyloxy, alkyl, cycloalkyl, a monocyclic or polycyclic (un)substituted ring system; N is O or 1], useful as antiinflammatory, immunomodulatory and antiproliferatory agents. The obtained compds. were screened in inhibition assay for dihydroorotate dehydrogenase (DHODH) activity. For instance, cyclopentene-1-carboxylic acid derivative II showed IC<sub>50</sub> value (human DHODH) of < 1μM.

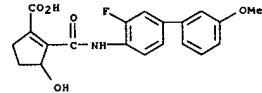
IT 717824-35-6P 717824-36-7P 719301-48-1P  
 719301-49-2P 719301-52-7P 719301-53-8P  
 719301-54-9P 719301-55-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

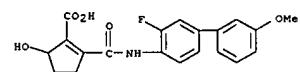
(preparation of cycloalkenedicarboxylic acid derivs., useful as antiinflammatory, immunomodulatory and antiproliferatory agents)

RN 717824-35-6 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]-3-hydroxy- (9CI) (CA INDEX NAME)

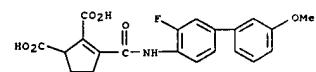
LS ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



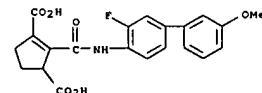
RN 717824-36-7 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 3-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 719301-48-1 CAPLUS  
 CN 2-Cyclopentene-1,2-dicarboxylic acid, 3-[(3-fluoro-3'-methoxy[1,1'-biphenyl]-4-yl)amino]carbonyl]- (9CI) (CA INDEX NAME)

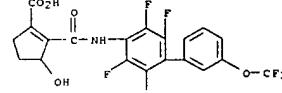


RN 719301-49-2 CAPLUS  
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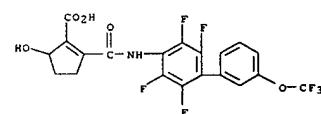


RN 719301-52-7 CAPLUS  
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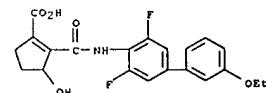
LS ANSWER 5 OF 6 CAPLUS COPYRIGHT 2006 ACS on STN (Continued)



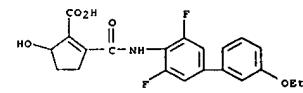
RN 719301-53-8 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 5-hydroxy-2-[(2,3,5,6-tetrafluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl)amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 719301-54-9 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3'-ethoxy-3,5-difluoro[1,1'-biphenyl]-4-yl)amino]carbonyl]-3-hydroxy- (9CI) (CA INDEX NAME)



RN 719301-55-0 CAPLUS  
 CN 1-Cyclopentene-1-carboxylic acid, 2-[(3'-ethoxy-3,5-difluoro[1,1'-biphenyl]-4-yl)amino]carbonyl]-5-hydroxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

ACCESSION NUMBER: 2003:981447 CAPLUS

DOCUMENT NUMBER: 140:246103

TITLE: Discovery of a novel series of DHODH inhibitors by a docking procedure and QSAR refinement  
AUTHOR(S): Leban, Johann; Saeb, Wael; Garcia, Gabriel;  
Baugerther, Roland; Kramer, Bernd  
CORPORATE SOURCE: Martinsried, 82152, Germany  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(1), 55-58

CODEN: BMCLB9 ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:246103

AB A novel series of DHODH (dihydroorotate dehydrogenase) inhibitors was developed based on a lead which was obtained by a docking procedure and a medicinal chemical exploration. The activity of the initial lead was improved by a QSAR method to yield low nanomolar inhibitors.

IT 669063-49-49 669063-57-42 669063-59-69

669063-68-79 669063-69-82 669063-70-19

669063-72-39

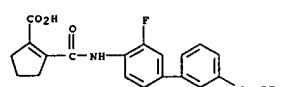
RL: PAC (Pharmacological activity); PFP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery of a novel series of dihydroorotate dehydrogenase inhibitors

by a docking procedure and QSAR refinement)

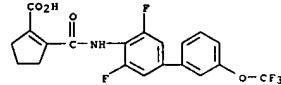
RN 669063-49-4 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[3-fluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



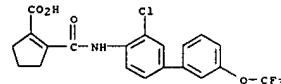
RN 669063-57-4 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[3,5-difluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

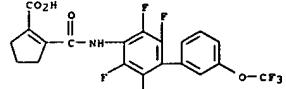


RN 669063-59-6 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[2,3,5,6-tetrafluoro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

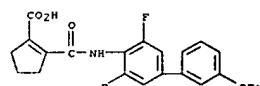


REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT



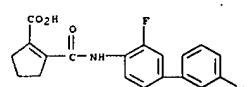
RN 669063-68-7 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[3'-ethoxy-3,5-difluoro[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



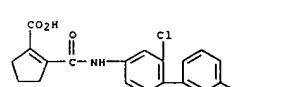
RN 669063-69-8 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[3-fluoro-3'-hydroxy[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 669063-70-1 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[2-chloro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)



RN 669063-72-3 CAPLUS

CN 1-Cyclopentene-1-carboxylic acid, 2-[[3-chloro-3'-(trifluoromethoxy)[1,1'-biphenyl]-4-yl]amino]carbonyl]- (9CI) (CA INDEX NAME)

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---Logging off of STN---

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Executing the logoff script...

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COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	31.58	200.05
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
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CA SUBSCRIBER PRICE	-4.50	-4.50

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